Neutron Reflection Conditions for Magnetic Lattice and Symmetry Operations

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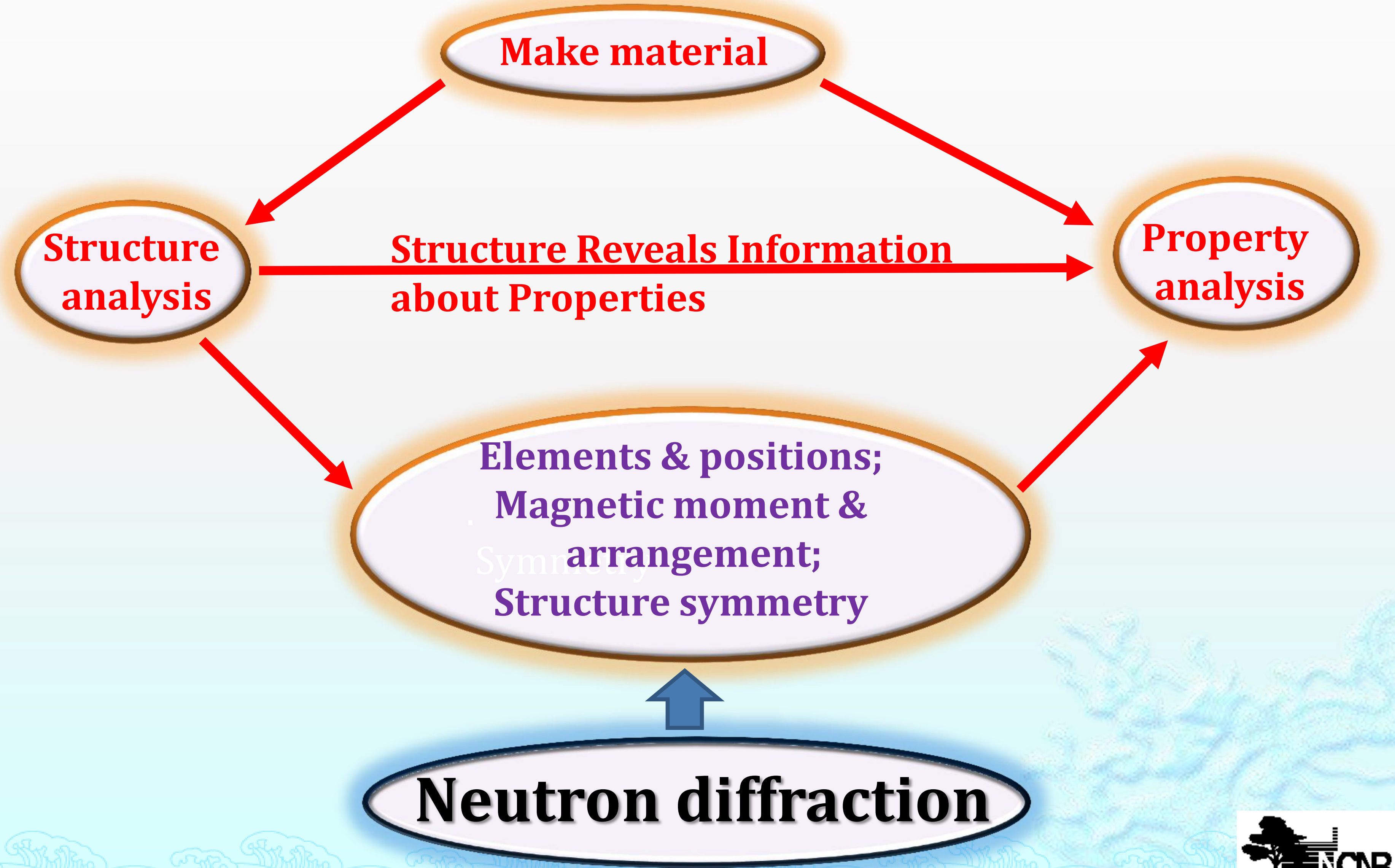
Outline

1. Structure of materials science;
2. Black and white magnetic lattices and symmetry operations
3. Reflection condition analysis;
4. Reflection conditions for magnetic lattices;
5. Reflection conditions for magnetic symmetry operations;
6. Discussion.

Structure in materials science



Structure determination from neutron powder diffraction for $K_{0.8}Fe_{1.6}Se_2$

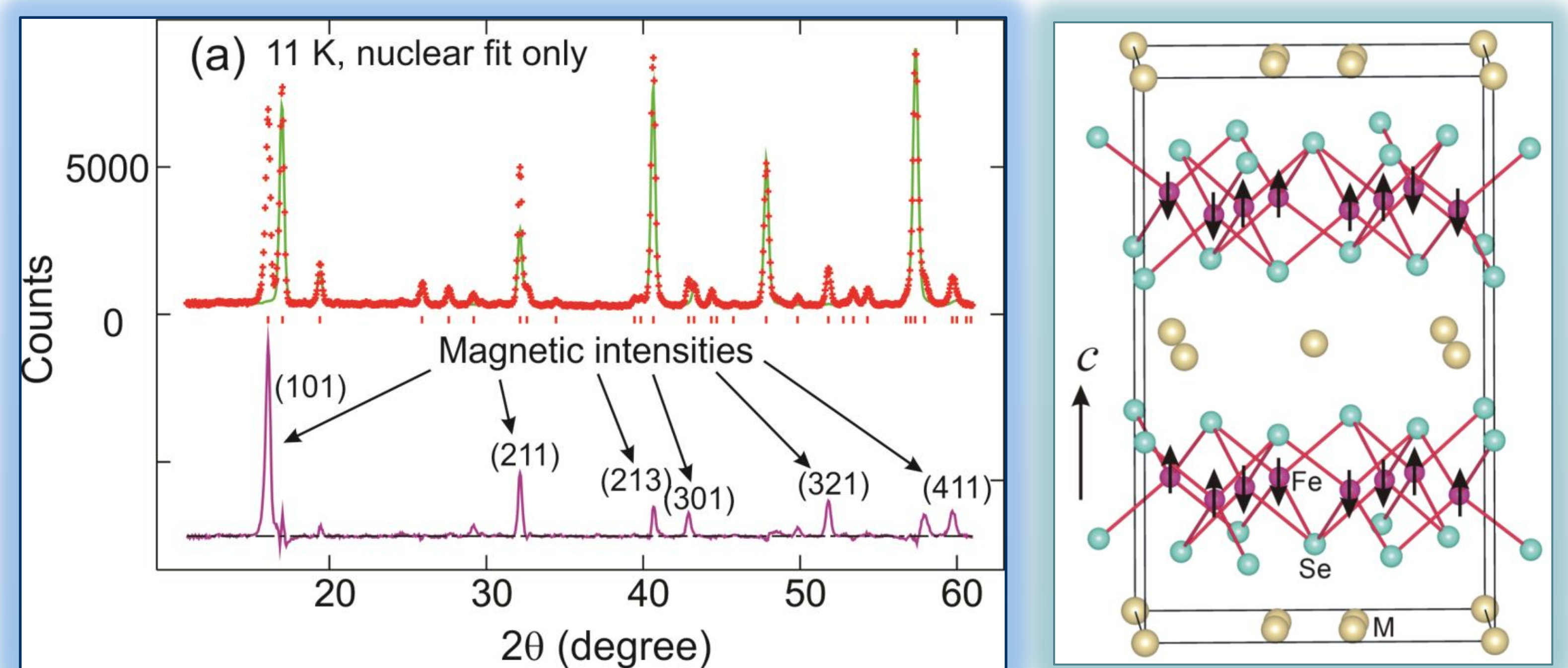


Fig. 1. (a) Neutron powder diffraction and (b) crystal and magnetic structures for $K_xFe_{2-x}Se_2$ superconductor. In (a), we have:

1) **Peak position:** $2d\sin\theta = n\lambda$;

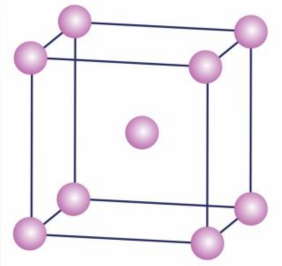
2) **Nuclear diffraction intensities**: $I_N = C\mathscr{M}_T[(\gamma e^2)/(2mc^2)]^2\ |F_N|^2$;

3) **Magnetic diffraction intensities**: $I_M = C\mathscr{M}_T\ A(\theta_B)\ [(\gamma e^2)/(2mc^2)]^2\ \langle 1-(\tau \cdot M)^2\rangle\ |F_M|^2$.

Magnetic reflection: ***h+k+l=2n, Body center?***

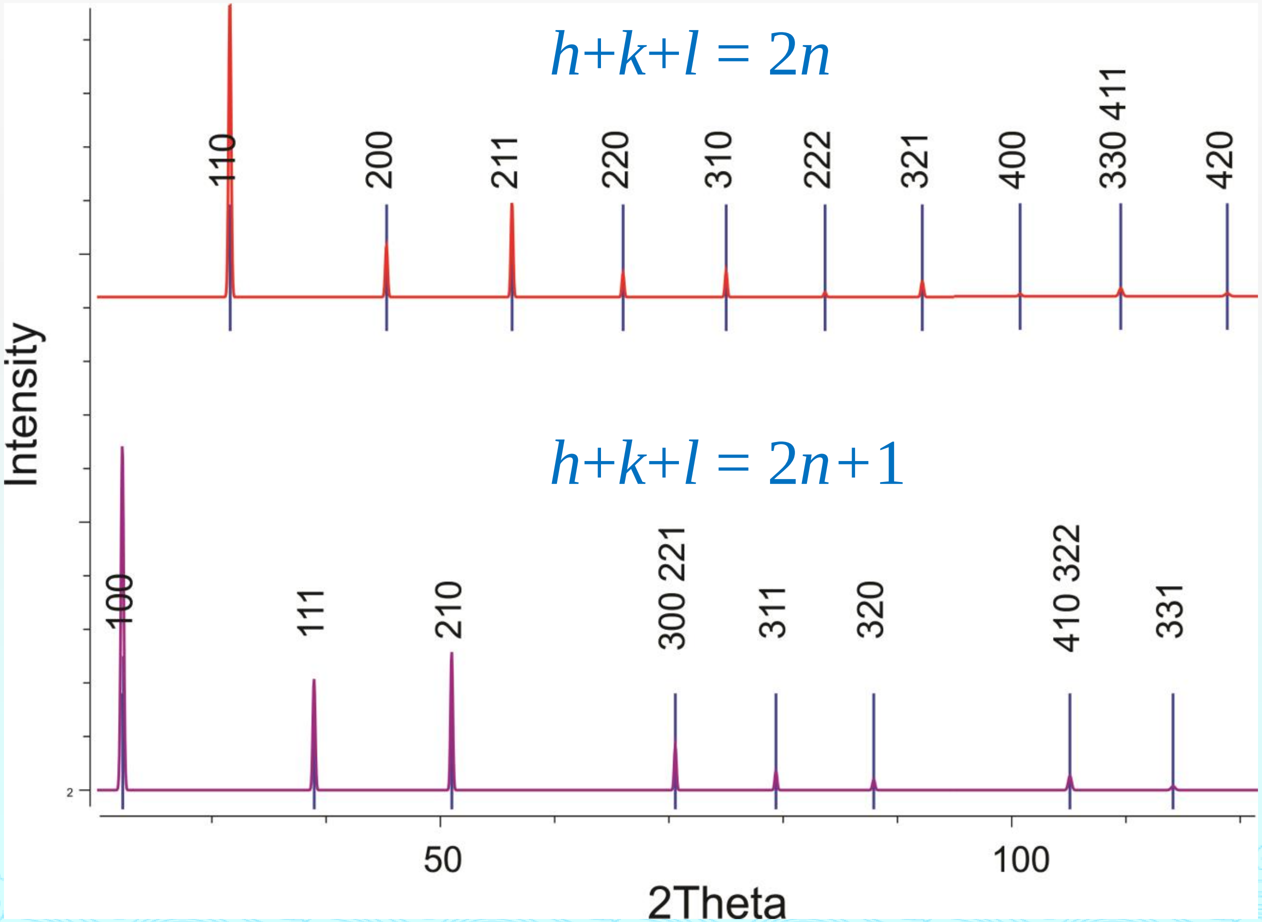
$$F_{hkl} = \sum p \exp(2\pi i(hx/a_0 + ky/b_0 + lz/c_0))$$

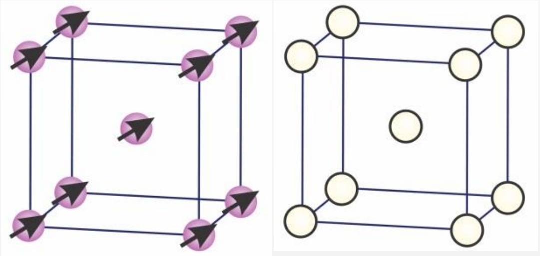
Determine reflection conditions from magnetic structure factor F_{hkl} calculations



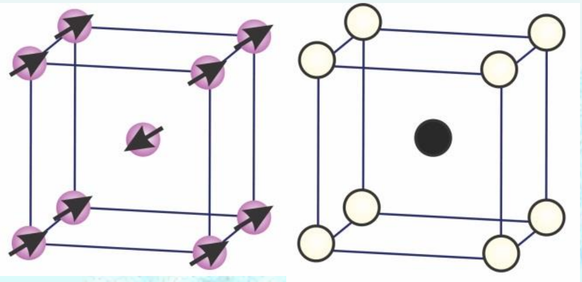
Nuclear
For $h\ k\ l$
$h+k+l = 2n$
Is known

$$F_{hkl} = \sum p \exp(2\pi i(hx/a_0 + ky/b_0 + lz/c_0))$$





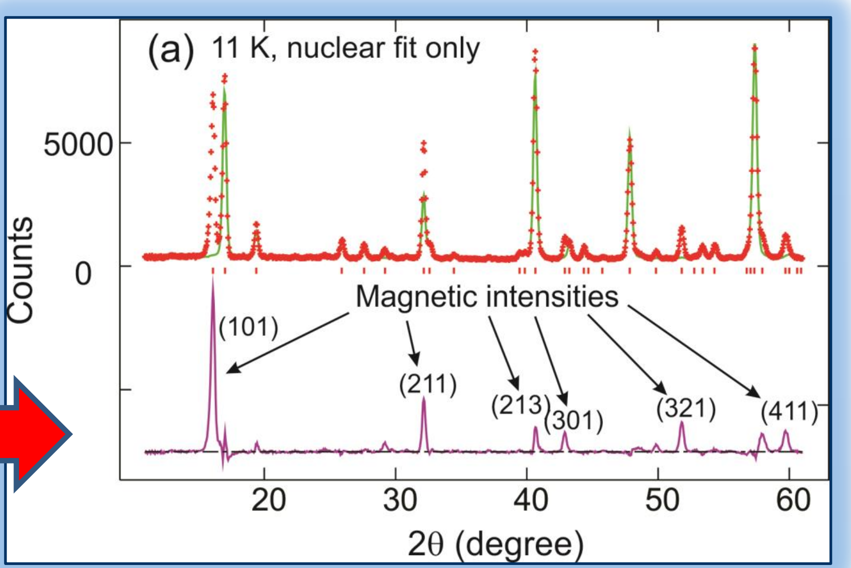
Ferromagnetic



Antiferromagnetic

Data collection and analysis

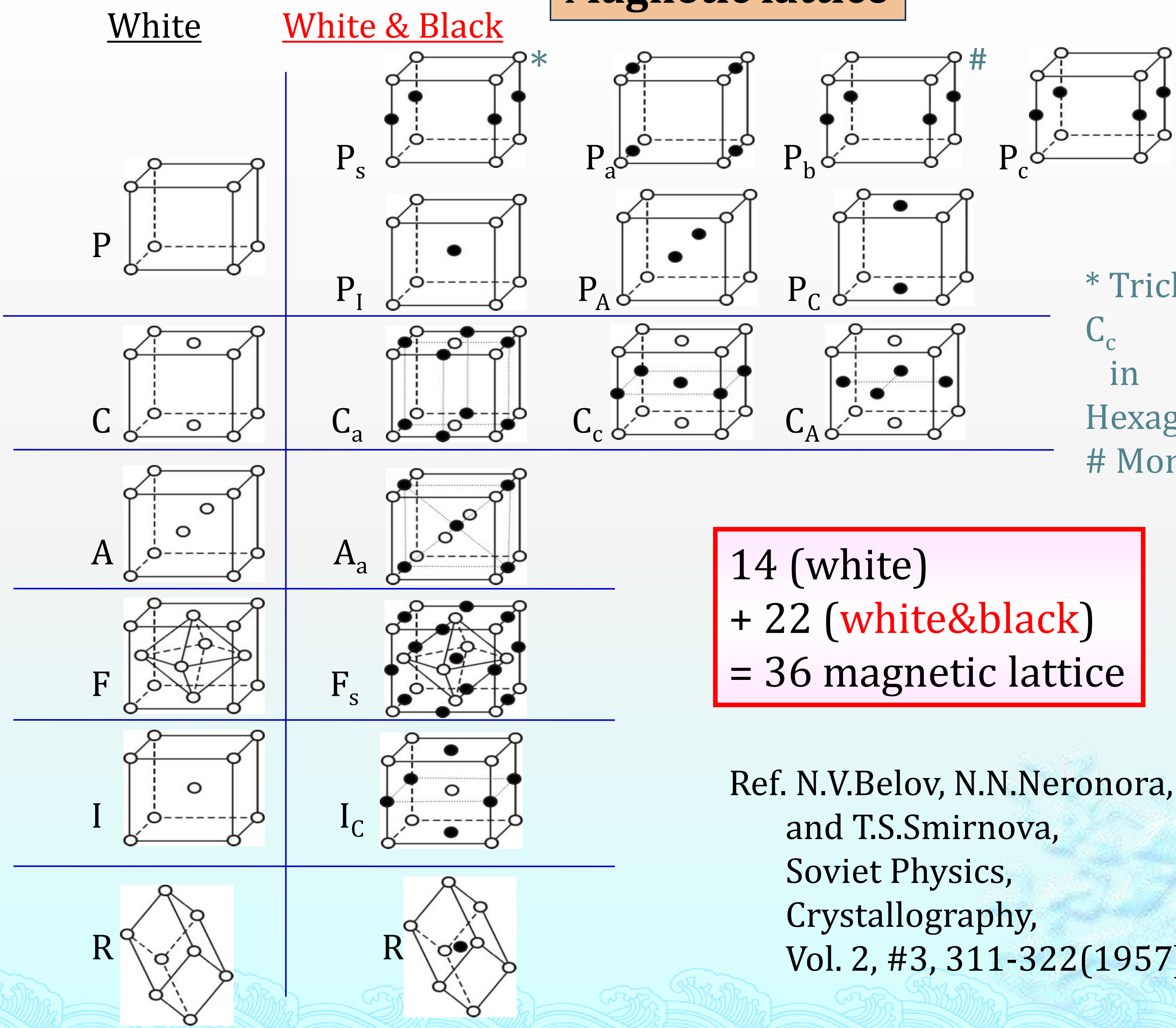
BT1 32-counter high-resolution
neutron powder diffractometer at NCNR



Data Analysis

GSAS- General Structure Analysis System

Magnetic lattice

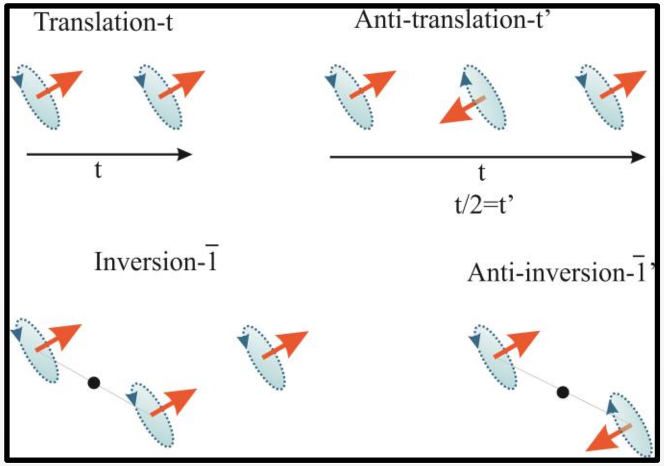


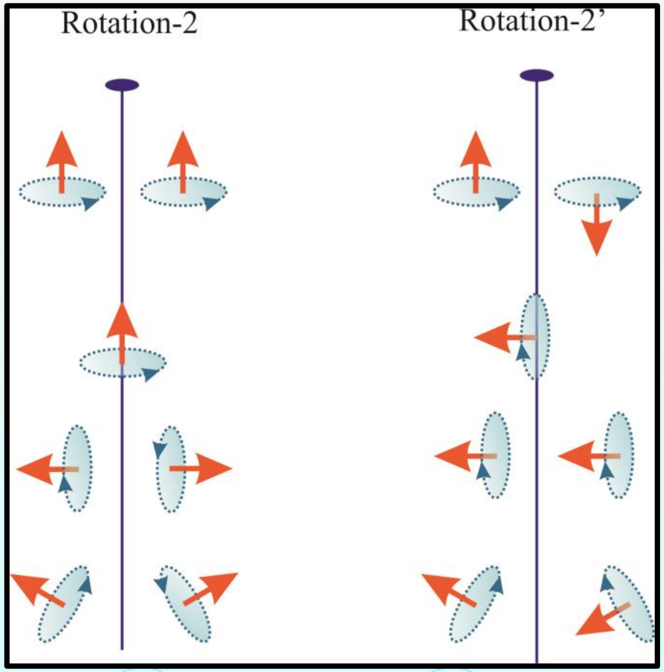
* Triclinic & C_c in Hexagonal
\# Monoclinic

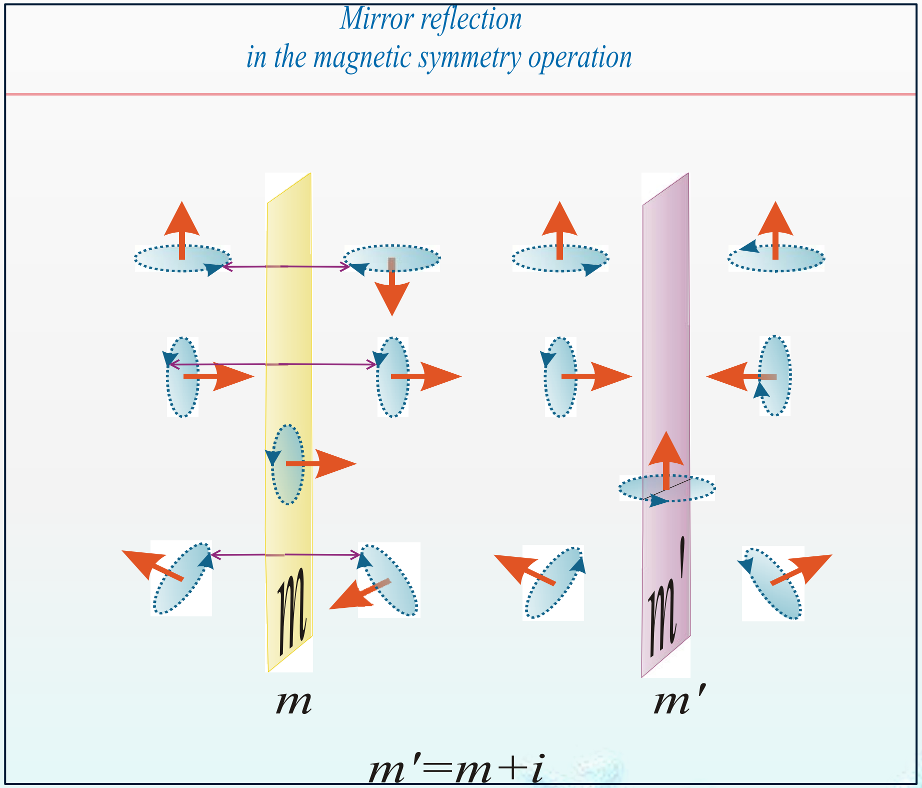
14 (white)
\+ 22 (white&black)
= 36 magnetic lattice

Ref. N.V.Belov, N.N.Neronora, and T.S.Smirnova, Soviet Physics, Crystallography, Vol. 2, #3, 311-322(1957)

Some magnetic symmetry operations

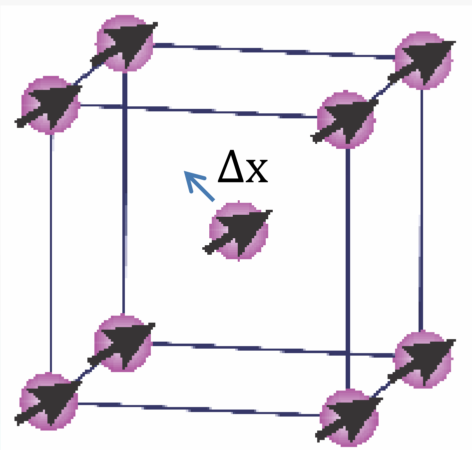


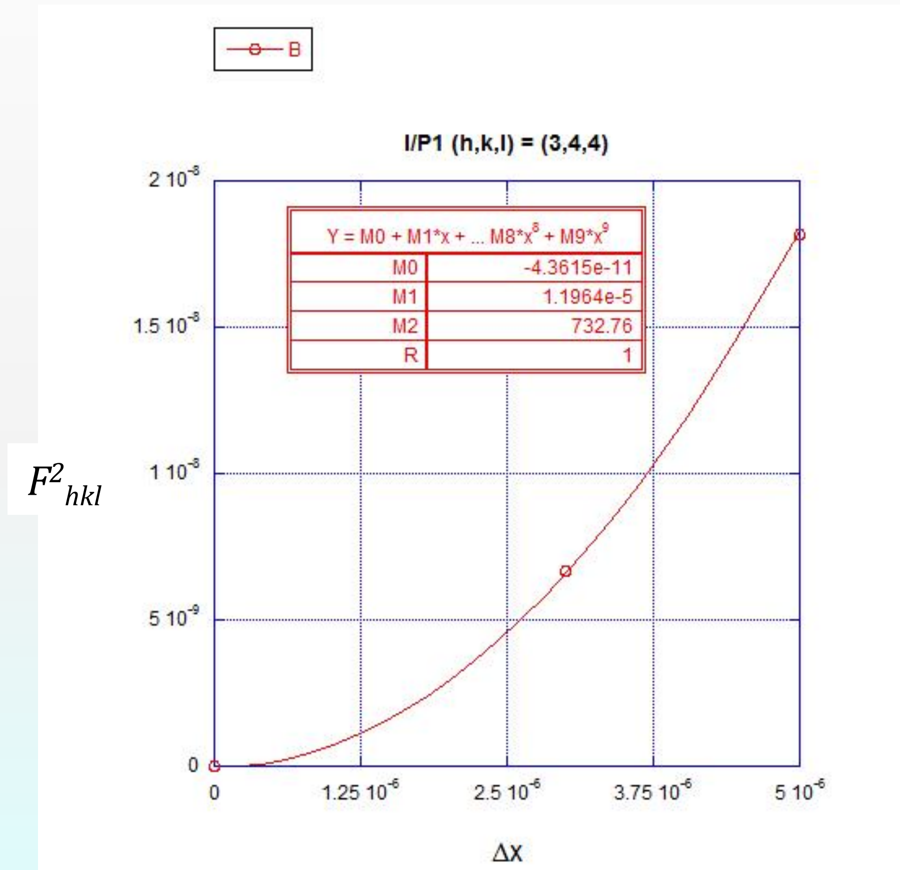




Reflection condition analysis

$$F_{hkl} = \sum p \exp(2\pi i(hx/a_0 + ky/b_0 + lz/c_0))$$

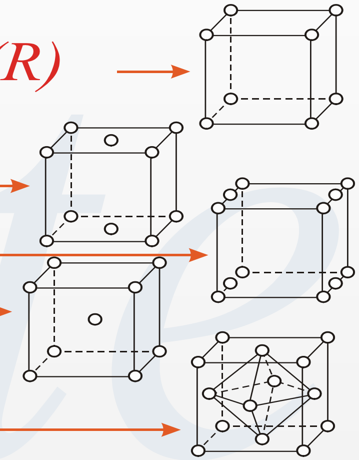




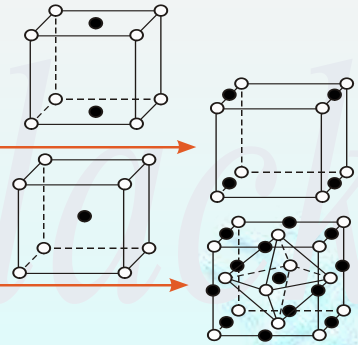
Simulations were done using GSAS. This is the graph of the maximum structure factor as a function of Δx. The threshold of 10^{-8} is passed at approximately $3.7\text{x}10^{-6}$.

Intergral reflection conditions for centred magnetic (white and black) cells (lattices).

Condition	type	Symbol
None	Primitive	P, R(R)
$-h+k+l=3n$	Primitive	R(H)
$h+k=2n$	C-face	C
$k+l=2n$	A-face	A
$h+k+l=2n$	Body center	I
h,k,l all odd or all even	Face center	F



Condition	type	Symbol
$h+k=2n+1$	Black C-face	P_C
$h=2n+1$	Black a-axis	P_a
$h+k+l=2n+1$	Body center	P_I
h,k,l all odd	Face center	F_s



White: Black; White &Black: Red

Reflection conditions for symmetry operations

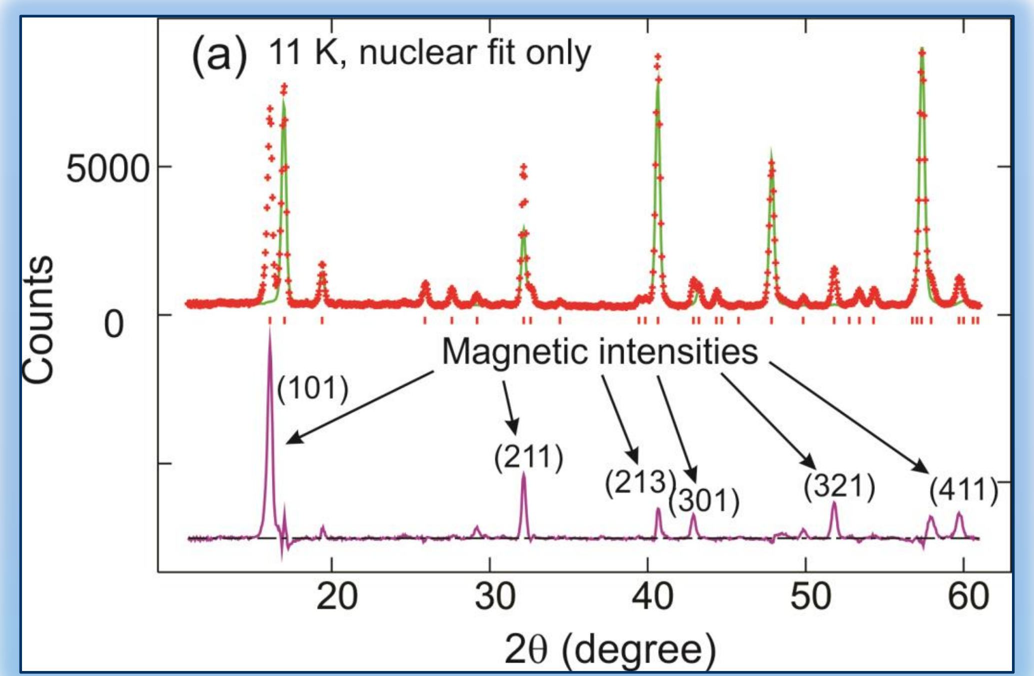
Symmetry Operation	Nuclear Reflection Condition	Magnetic Reflection Condition*
a (a-glide)	$k + l = 2n$	None
b (b-glide)	$h + l = 2n$	None
c (c-glide)	$h + k = 2n$	None
2_1	$0k0$: $k = 2n$	$0k0$: $k = 2n + 1$
$2'_1$	--	$0k0$: $k = 2n$

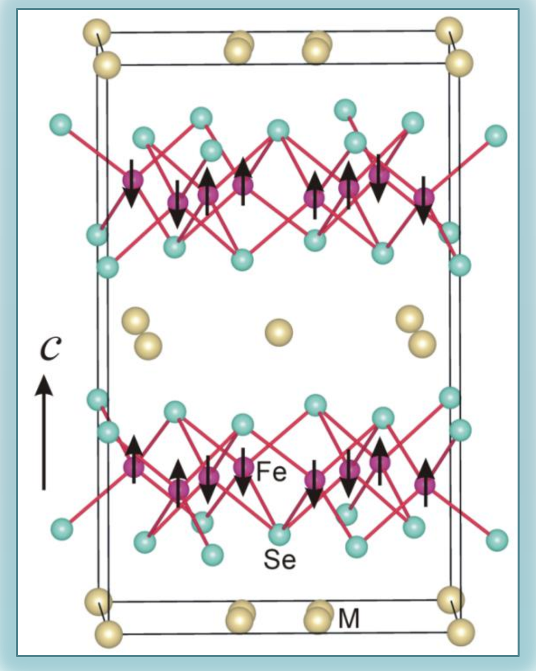
Reflection conditions for symmetry operations

Symmetry Operation	Nuclear Reflection Condition	Magnetic Reflection Condition*
4_i (i=1, 3)	00*l*: $l = 4n$	00*l*: $l = 2n+1$
$4'_i$ (i=1, 3)	--	00l: $l = 2n+1$
3_i (i = 1, 2)	00*l*: $l = 3n$	00*l*: $l \neq 3n$
6_i (i = 1, 5)	00*l*: $l = 6n$	00*l*: $l = 2n + 1 \neq 3$n

- *For the symmetry operations where the lattice is left ferromagnetic, the magnetic reflection conditions are the same as the nuclear reflection conditions

Magnetic symmetry for $K_{0.8}Fe_{1.6}Se_2$: *I4/m'*

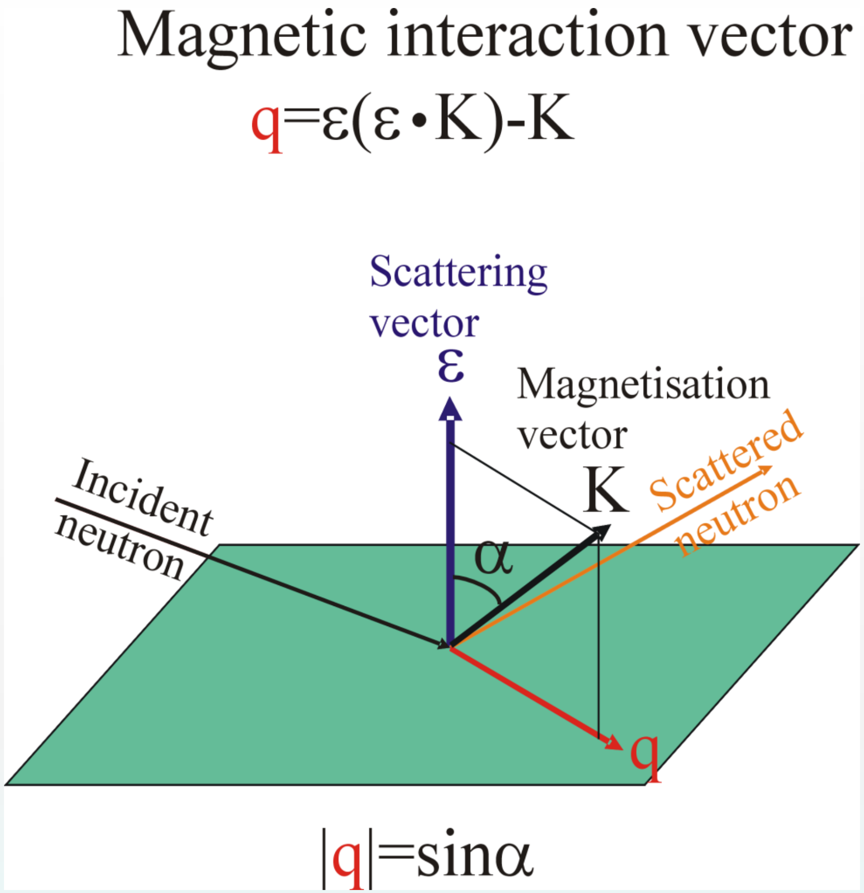




Magnetic reflection condition for (*h k l*): *h+k+l=2n,*

Body center lattice

I(001)=0, Why?



Moments //c-axis
α=0, i.e sinα=0
I(00l)=0,

Further work

- Change in magnetic moment amplitude
- Change in magnetic moment orientation
- Confirm results by analyzing F^2 formula

Acknowledgements

Thanks to

- Qing Huang
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- Dan Neumann
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